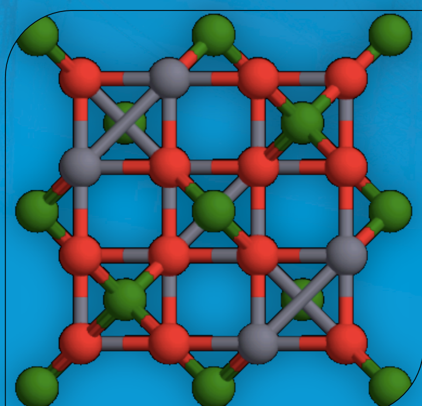
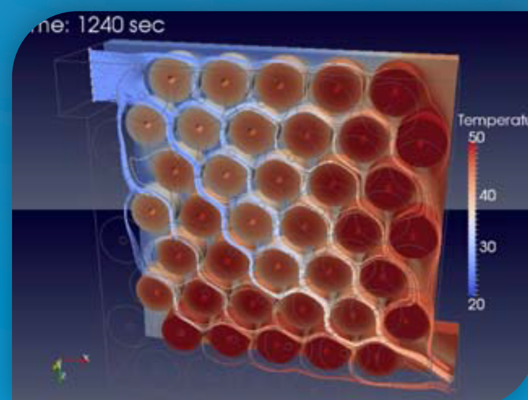
SFU NRC·CNRC

Succeeding With New Energy Materials:
A MARKET-DRIVEN MODELING APPROACH

Kourosh Malek
ICTP, Trieste, Italy
July 04, 2016





College on Multi-scale Computational Modeling of Materials for Energy Applications

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2014 **$7B**

2023 **$19B**

Source: Navigant Research, 2015

Market Acceptance

- Safety
- Codes & Standards
- Performance
- Policy

Cost

- Materials Cost
- Manufacturing processes
- System Integration

Durability

- Materials Degradation
- Operational / Integration Challenges

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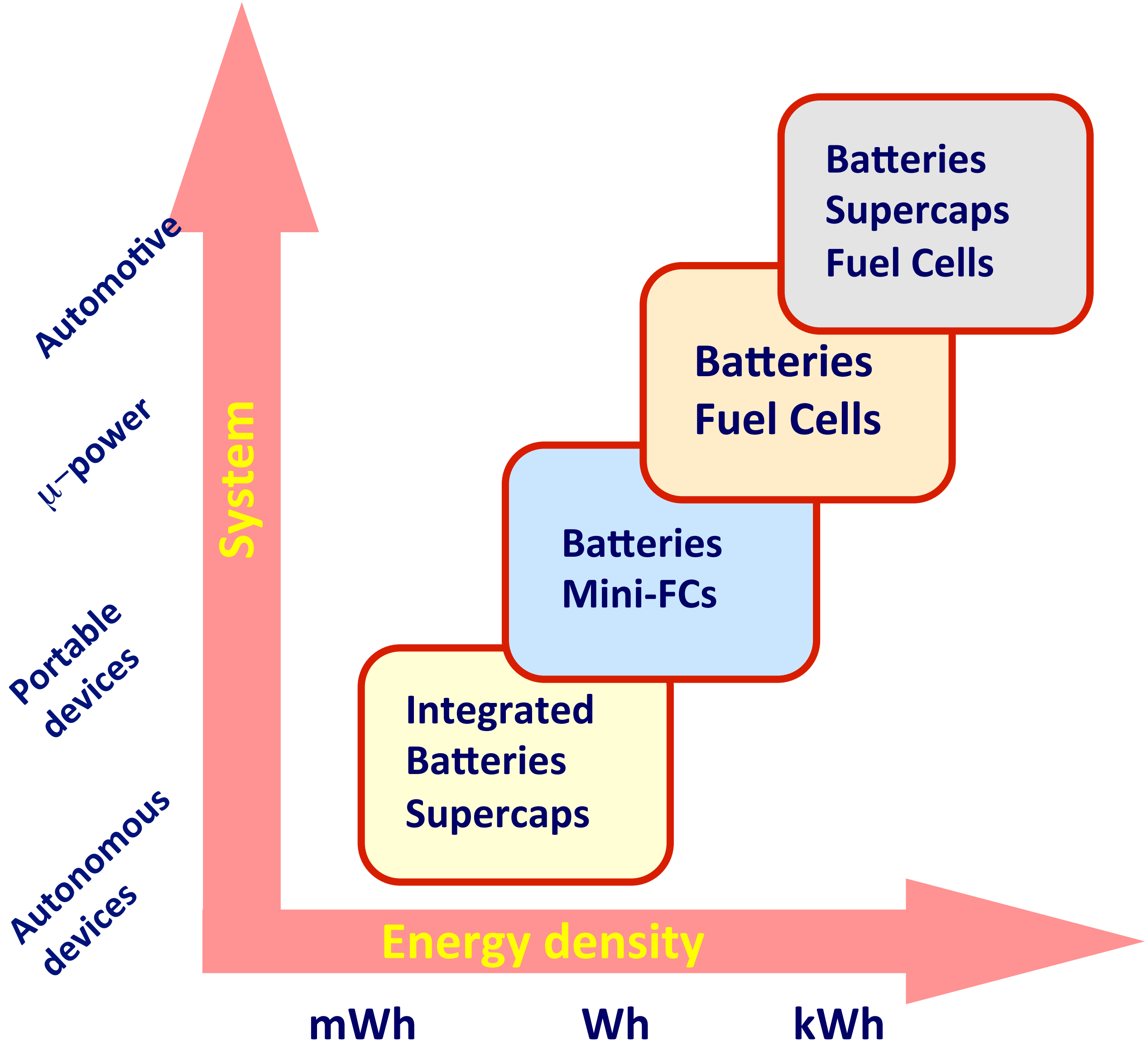

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Objective

Introducing a cost assessment platform dedicated to electrochemical materials

- Technical performance targets -> application area
- Cost of production (lab to market)
- Market assessment

DIRECTED TECHNOLOGIES INC.

SA STRATEGIC ANALYSIS

TIAX

BOOTHROYD DEWHURST, Inc. DFMA®

Modeling approaches

- Materials simulation and modeling
- Production scale up of R&D (Techno-economic Cost Model-TCM)
- Investment Methodology of Materials (IMM)

Technical Performance

Cost of Production

Market Value

Investment Potential

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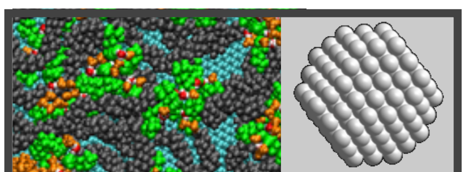
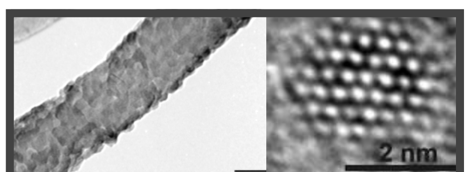
Materials Design by Modeling



Materials Modeling
Simulation



Fabrication
Characterization

Integration & Testing
Commercialization

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Design Challenges

Materials Modeling

Accelerate material characterization	Improve critical reactions	Design with optimized properties	Understand key processes

Nanostructure Materials

- Energy Storage and Conversion
  - Photovoltaics
  - Batteries Capacitors
  - Fuel Cells
- Catalysts Membranes
- Materials for Harsh Environment
- Electronics and Sensors

FOREMOST OBJECTIVE

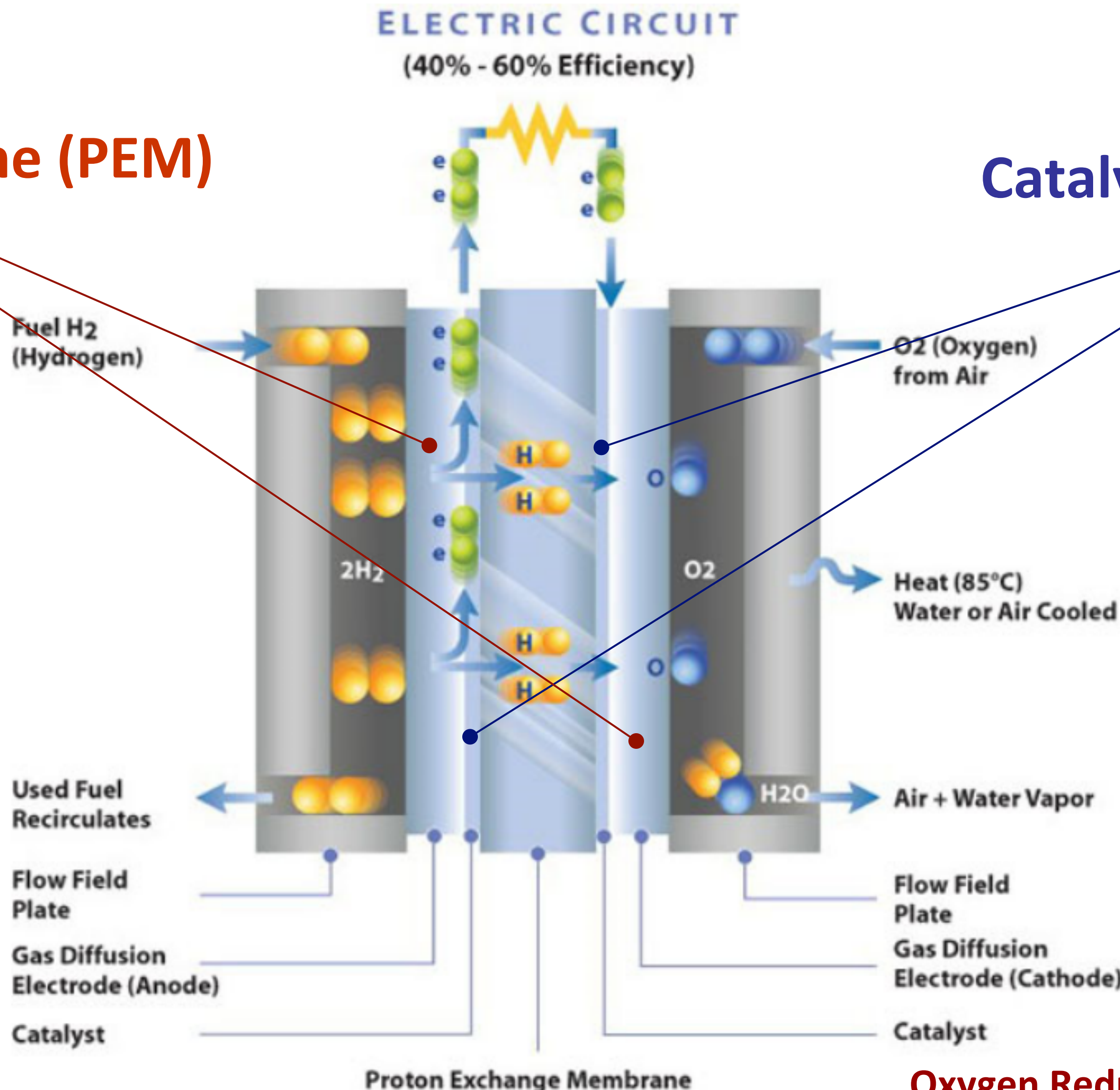
Maximum function at given cost and lifetime

Polymer Electrolyte Fuel Cells

Membrane (PEM)

Catalyst layers (CL)

MEA



Ballard Power System

Oxygen Reduction Reaction (ORR)
Hydrogen Oxidation Reaction (HOR)

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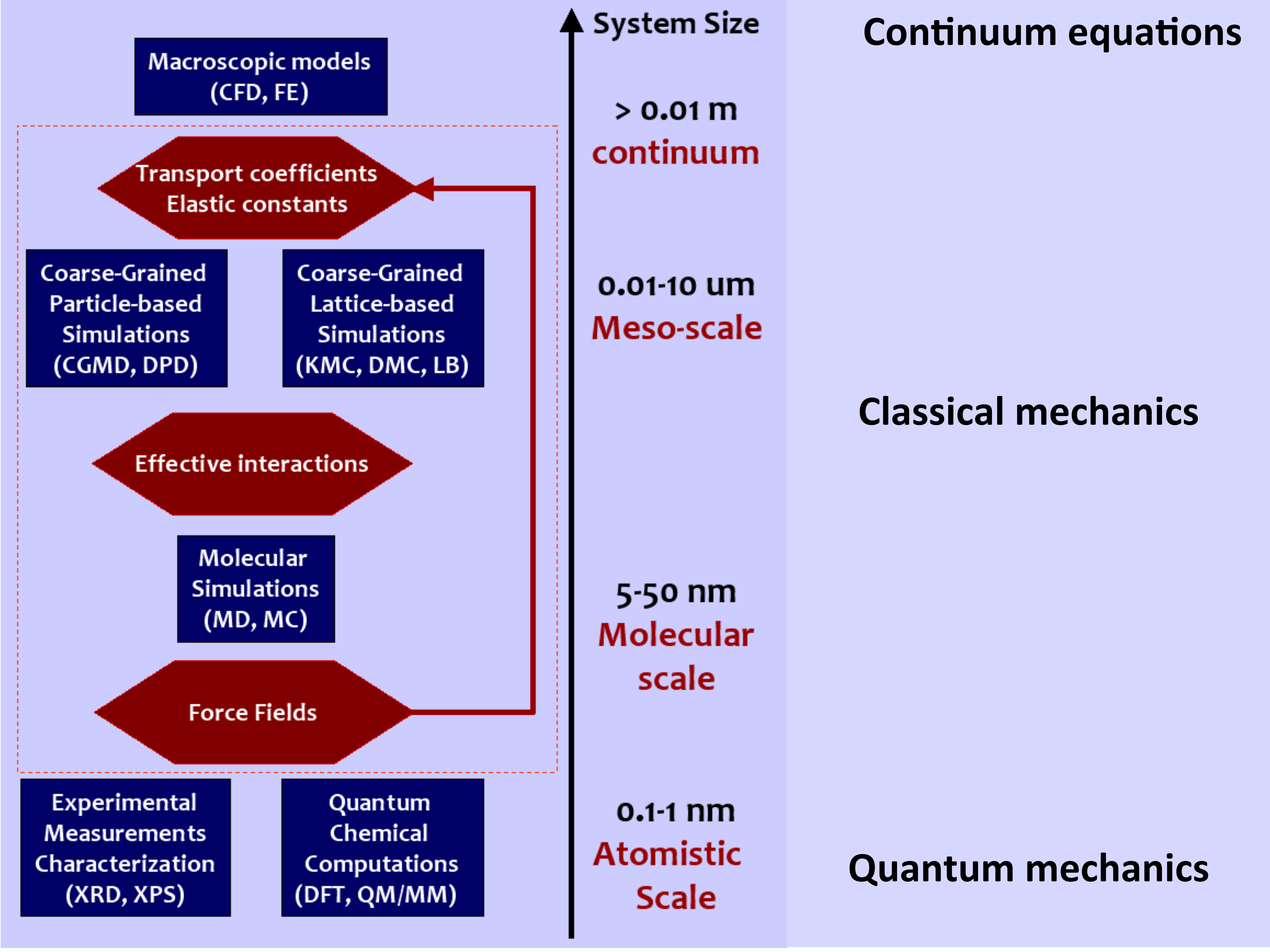
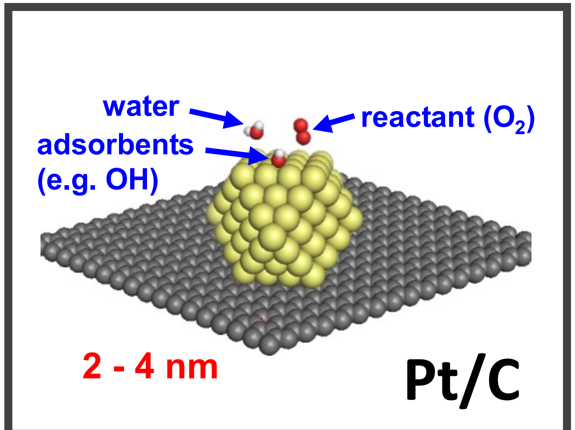
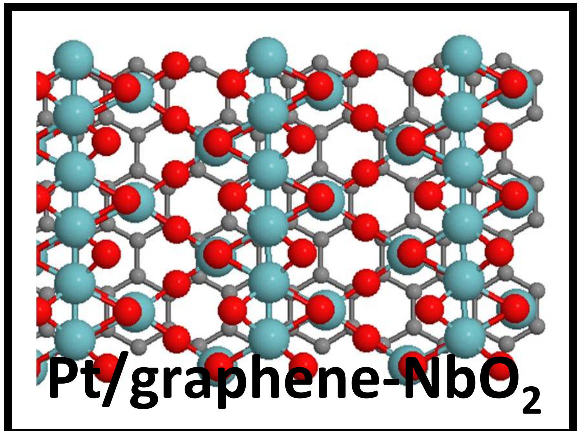

System Size
Macroscopic models (CFD, FE)
Transport coefficients
Elastic constants
Coarse-Grained Particle-based Simulations (CGMD, DPD)
Coarse-Grained Lattice-based Simulations (KMC, DMC, LB)
Effective interactions
Molecular Simulations (MD, MC)
Force Fields
Experimental Measurements Characterization (XRD, XPS)
Quantum Chemical Computations (DFT, QM/MM)
> 0.01 m
continuum
0.01-10 um
Meso-scale
5-50 nm
Molecular scale
0.1-1 nm
Atomistic Scale
Continuum equations
Classical mechanics
Quantum mechanics

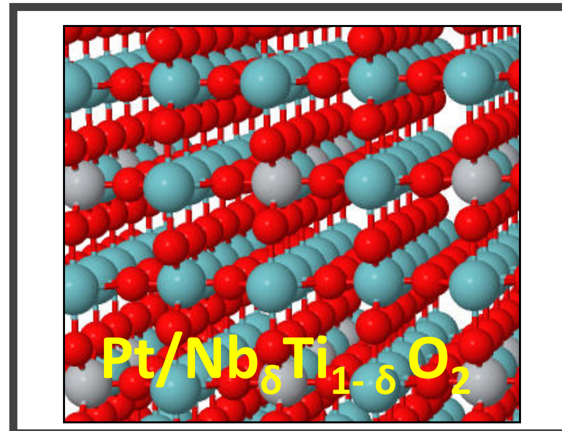
Modeling Electrochemical Materials



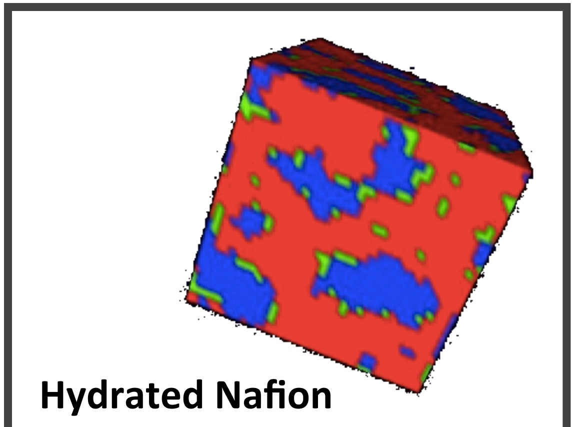
Electrodes



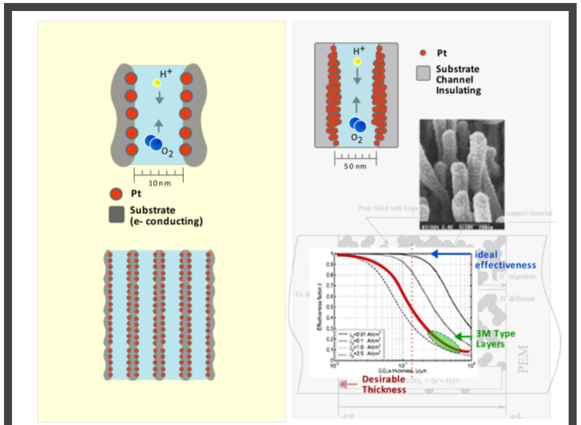
Nanostructured CL



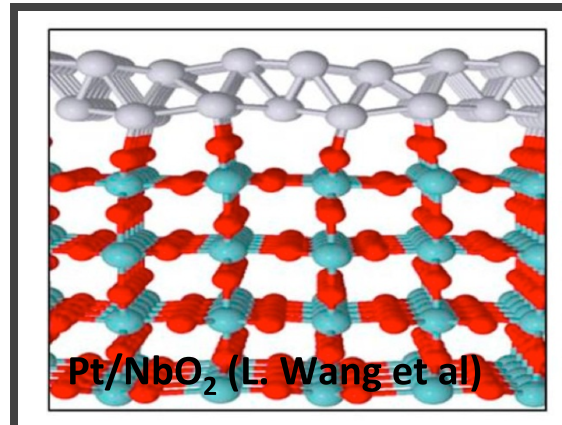
Support materials



Polymer membranes



Nanostructured CL



Support materials

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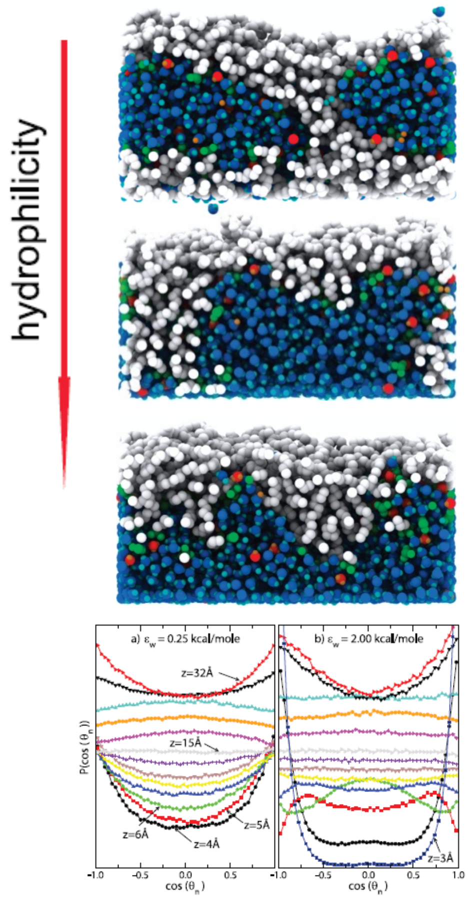
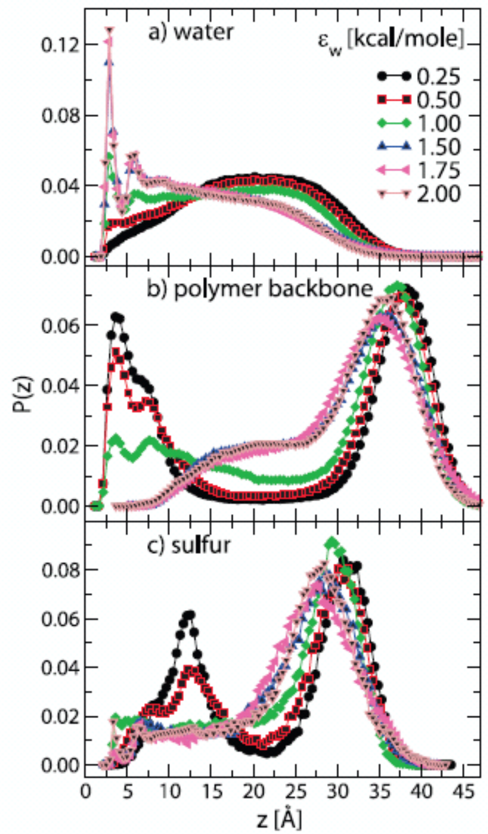
Catalyst layer of PEFC

Interfacial structure and processes

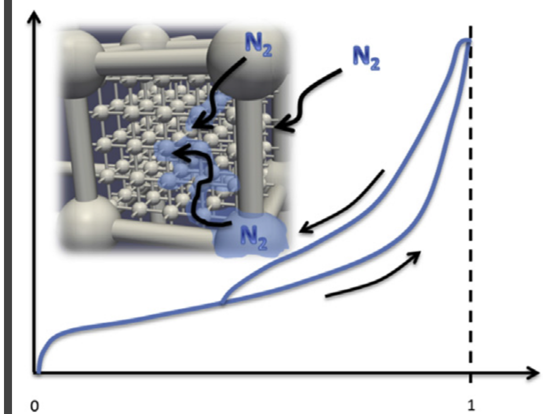


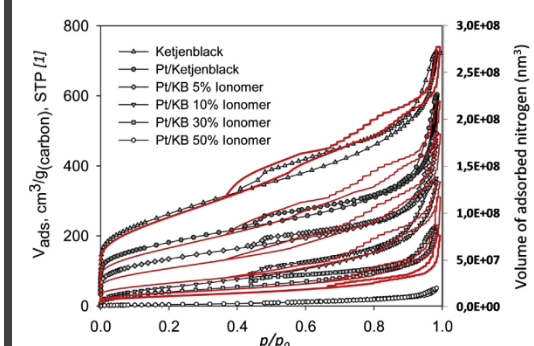
Interfacial properties



ACSNano, 2013

Interfacial properties





JPS, 2013

Porous CL

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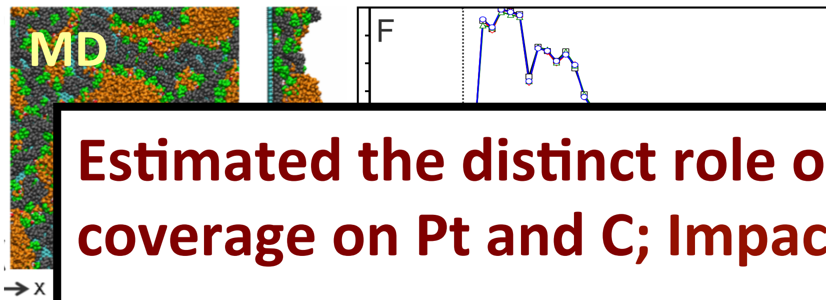
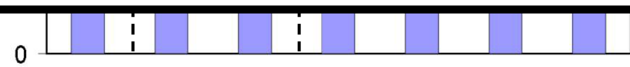
Catalyst layer of PEFC

Interfacial structure and processes

Ionomer → microstructure → ORR



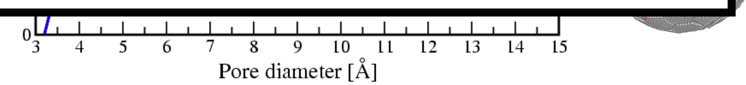
DI



T. Mashio et al., JPC-C 2010

Effect of ionomer on ORR (MD, DFT)

Effect of carbon support



Carbon 2011; JPS 2012

Effect of carbon model (MD)

Estimated the distinct role of ionomer content on ionomer coverage on Pt and C; Impacts on ORR activity

- **Method:** MD, CGMD, DFT, kinetics modeling
- **Characterization:** SANS, SAXS, CV, EIS
- **Impact:** vital for design of new generation CLs, pre-competitive knowledge

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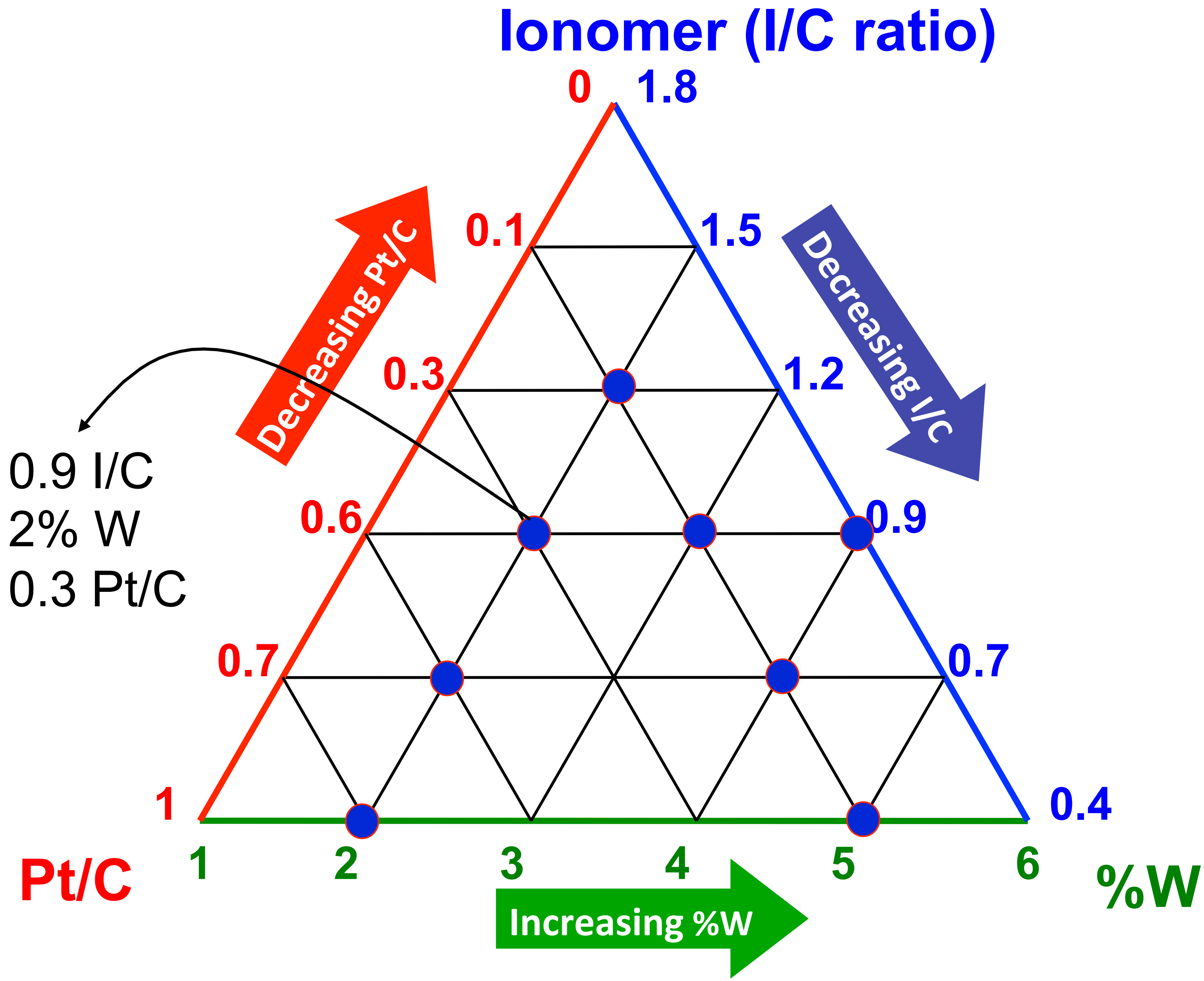
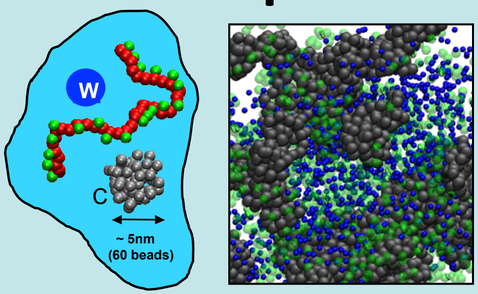

Ionomer (I/C ratio)
0
1.8
0.1
1.5
0.3
1.2
0.6
0.9
0.7
0.7
1
0.4
Decreasing Pt/C
Decreasing I/C
0.9 I/C
2% W
0.3 Pt/C
Pt/C
1
2
3
4
5
6
%W
Increasing %W

Advanced CL design

Step I	Step II	Step III
Model Development	**Model Refinement**	**Model Validation**

Step I

Model Development

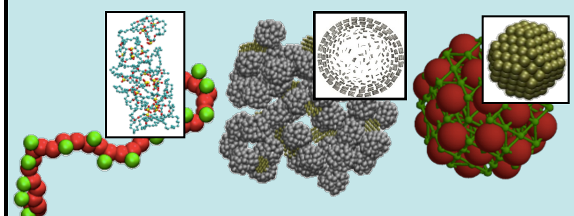


Effect of solvent
(implicit solvent, Pt)

Versatile CGMD
Ionomer-free aggl.
Phase segregation

Step II

Model Refinement

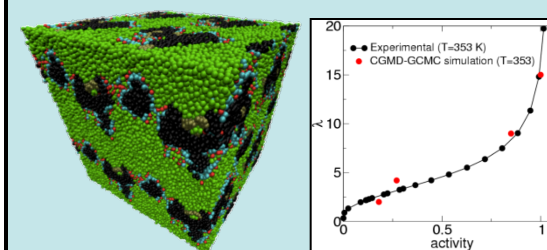


C → Pt/C
(explicit Pt)

CGMD → Physical model
→ Experimental data

Step III

Model Validation



Composition-microstr.
(characterization)

Water/gas ads.
Ionomer network
Water transport
Re-draw structural picture

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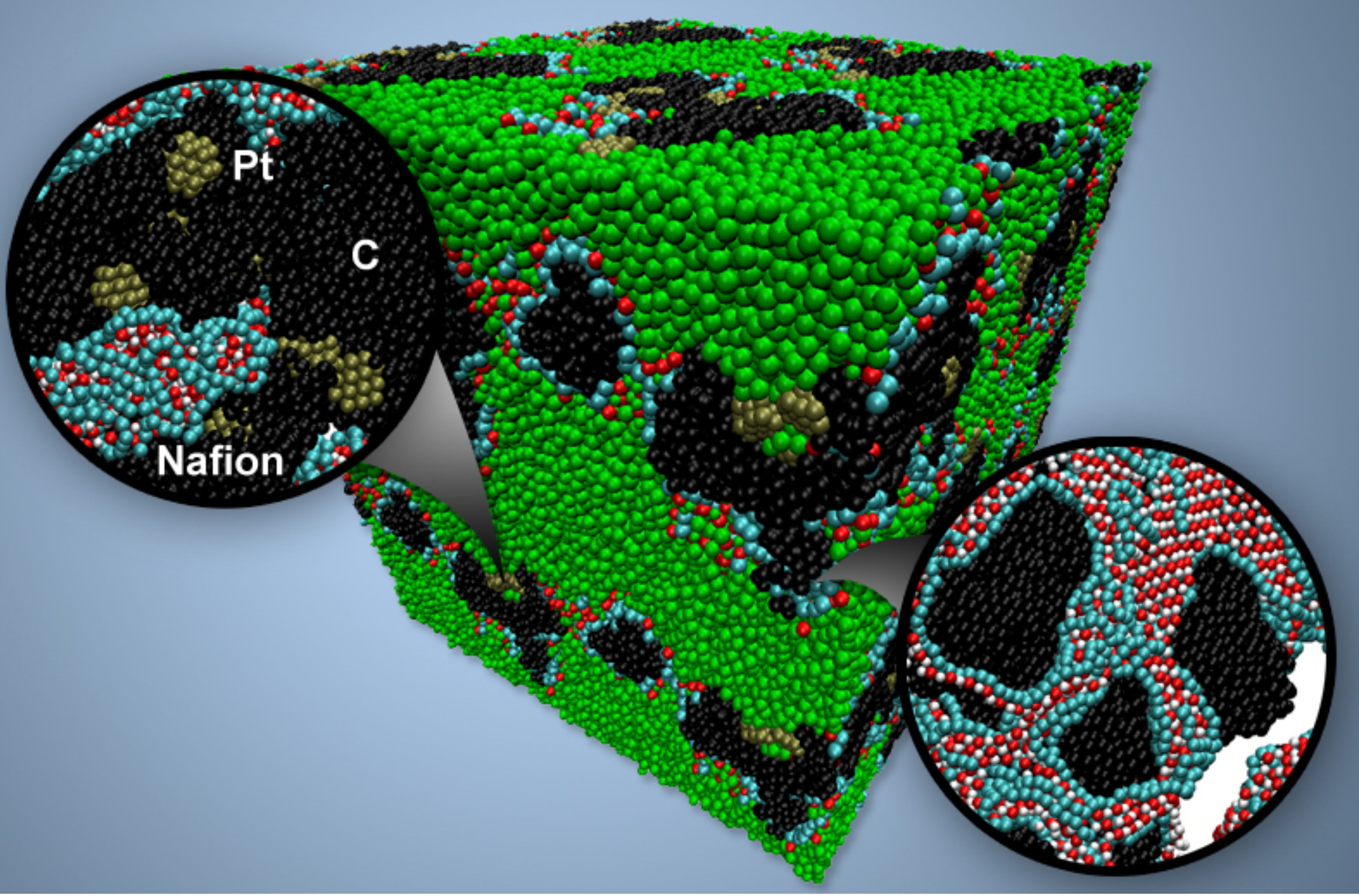
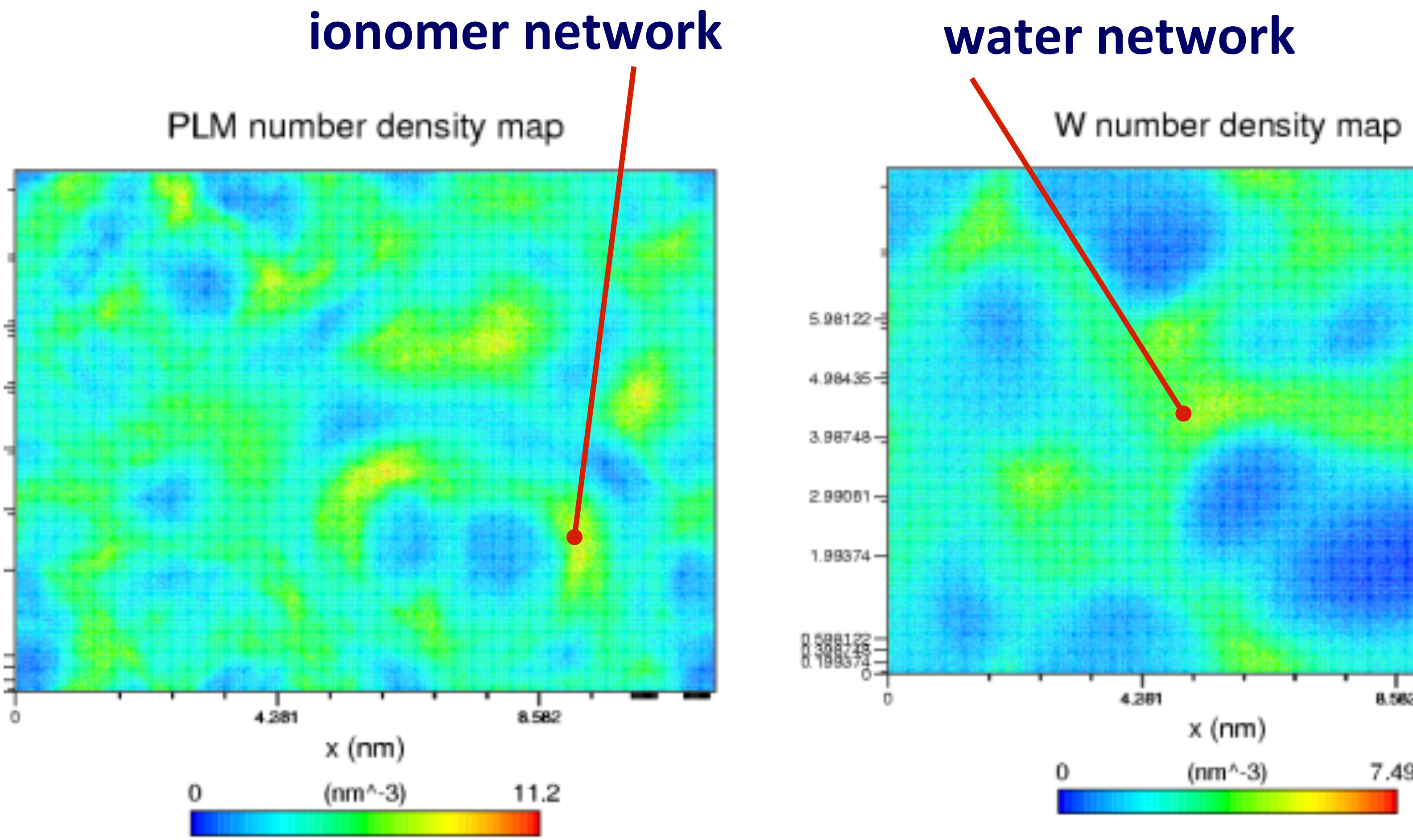


CL microstructure formation

Nafion-water structure



JPC 2007; JCP 2009; Electrocatalysis 2012

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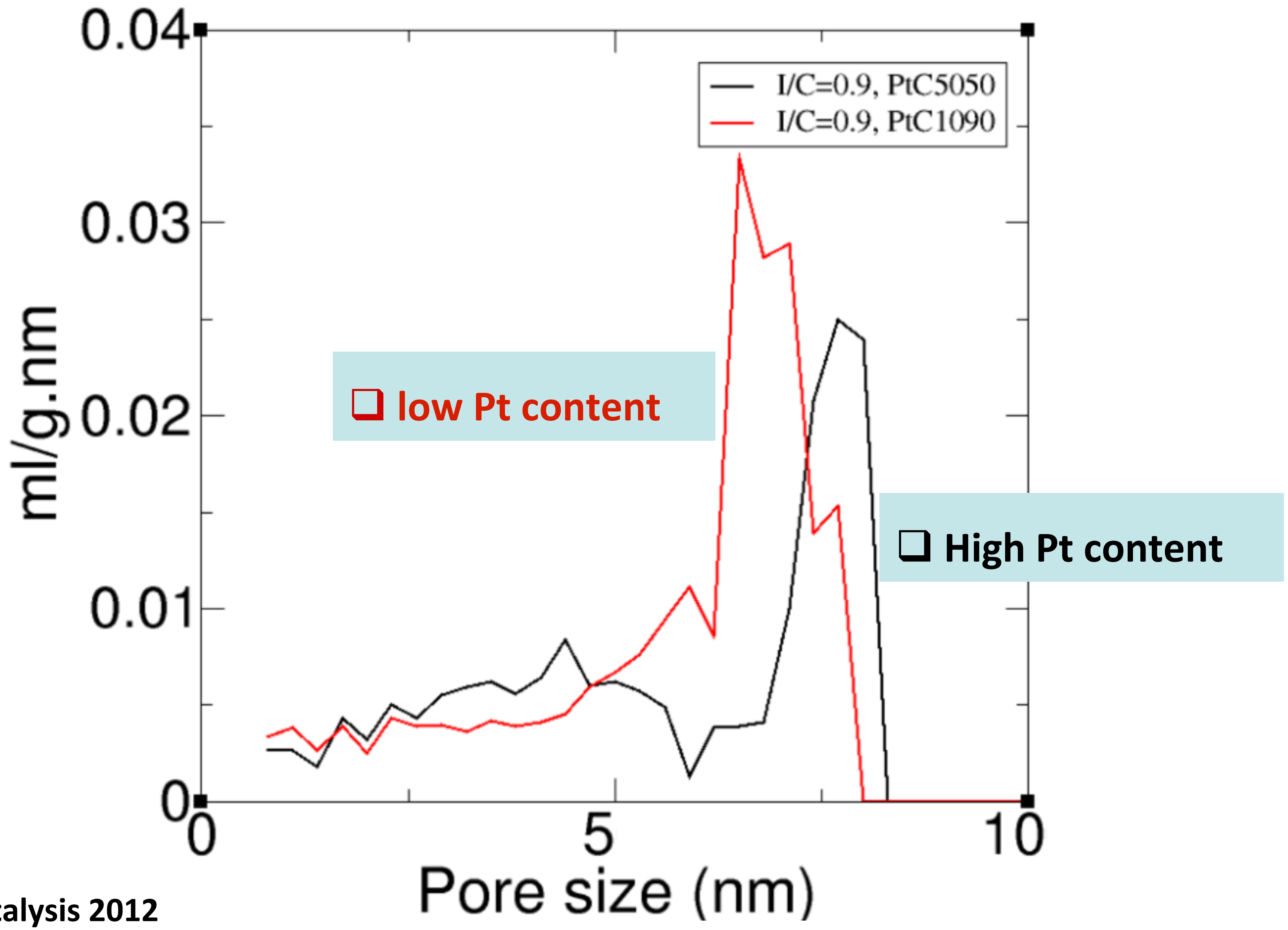
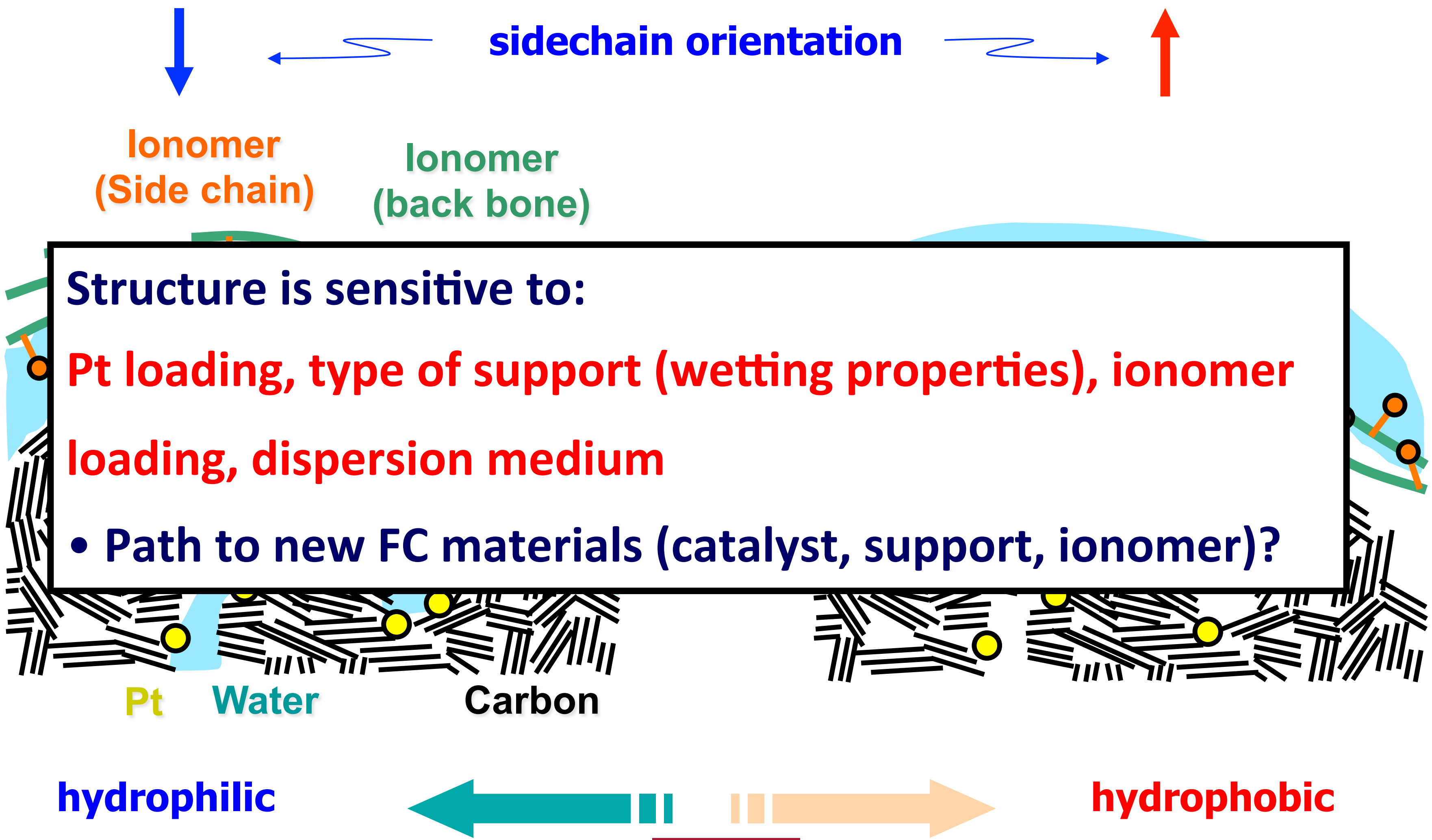
PSD: role of Pt



Electrocatalysis 2012

CL structural picture redefined!



Structure is sensitive to:

Pt loading, type of support (wetting properties), ionomer loading, dispersion medium

- **Path to new FC materials (catalyst, support, ionomer)?**

Cost assessment

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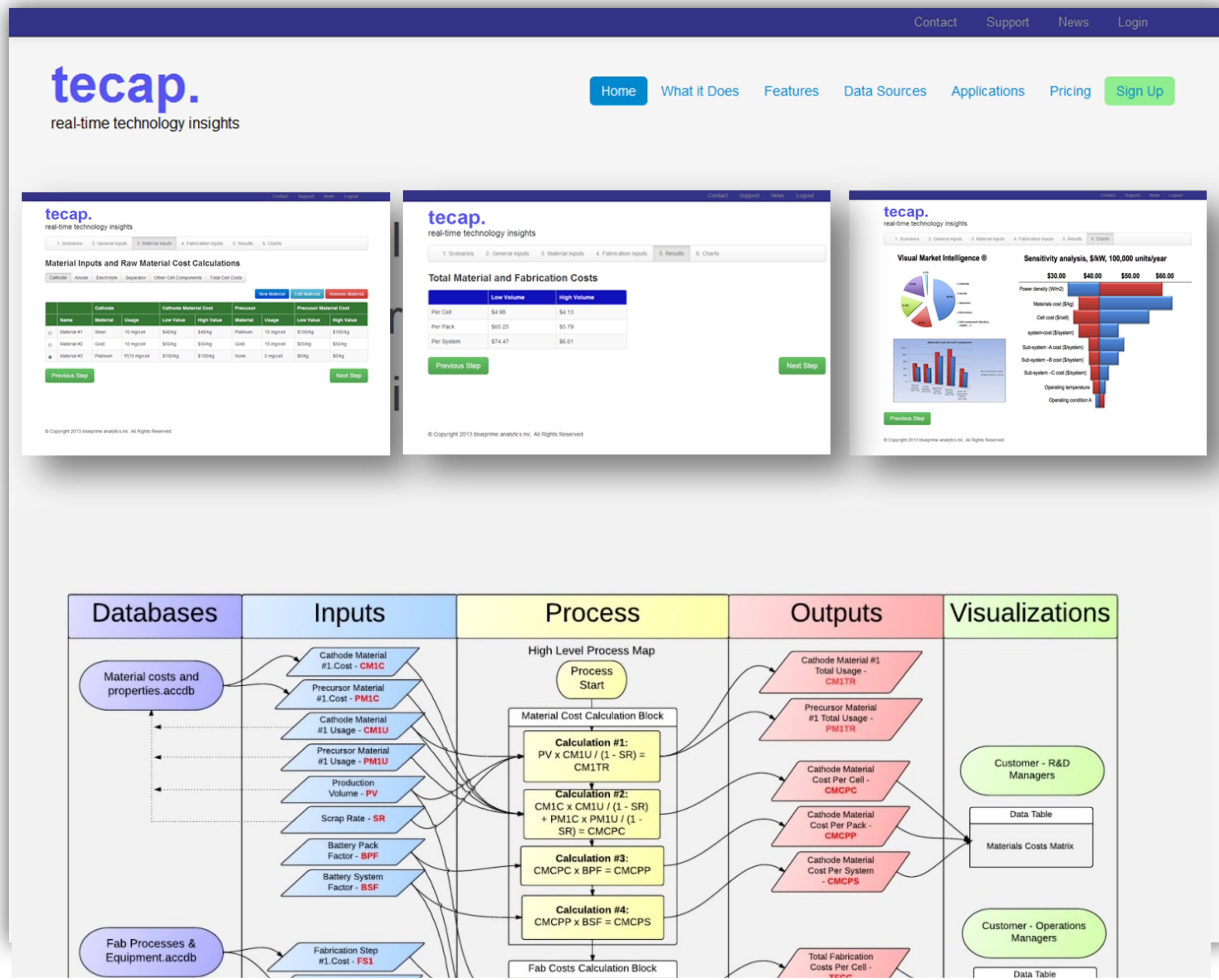
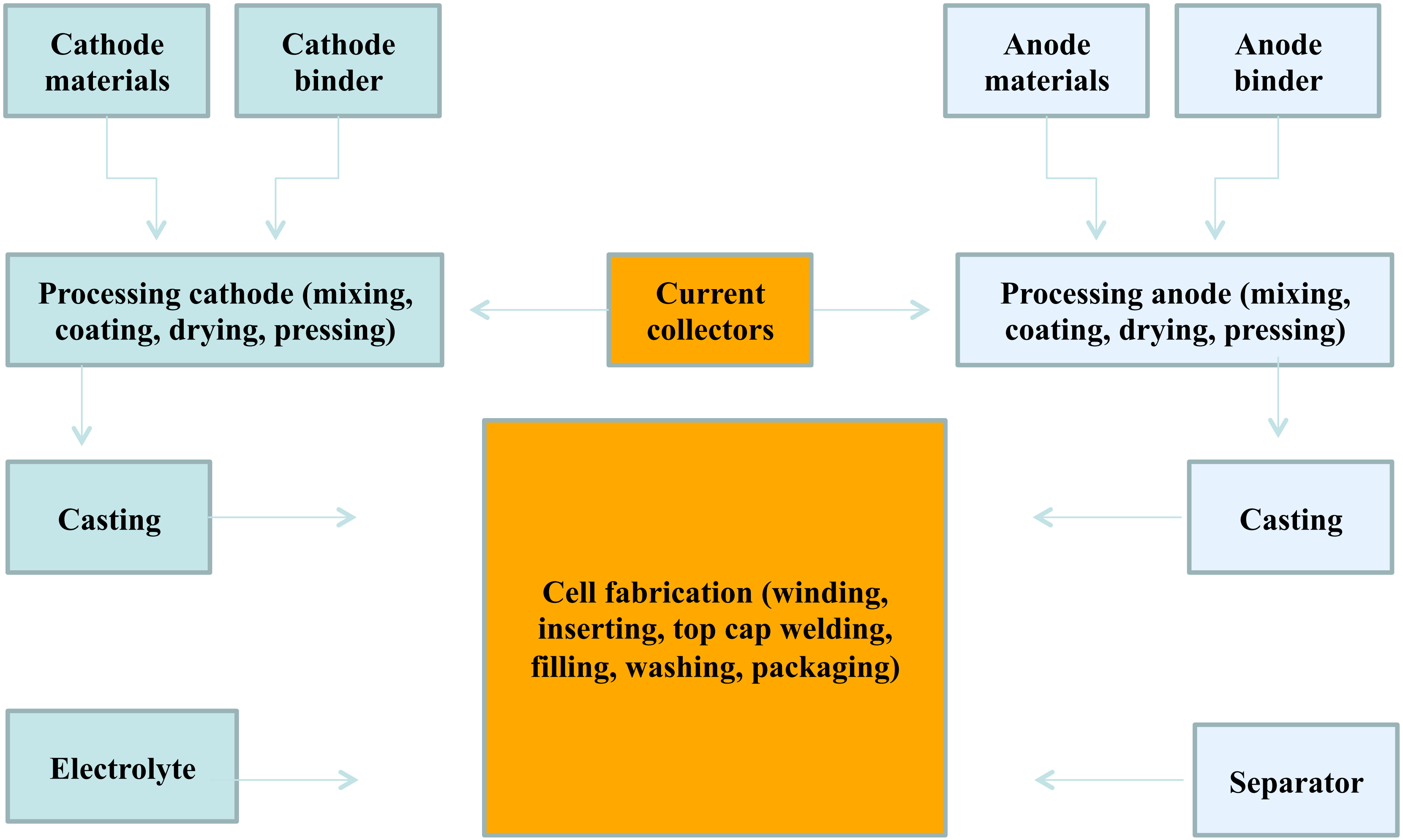
Process flow



TCM application: ES technologies



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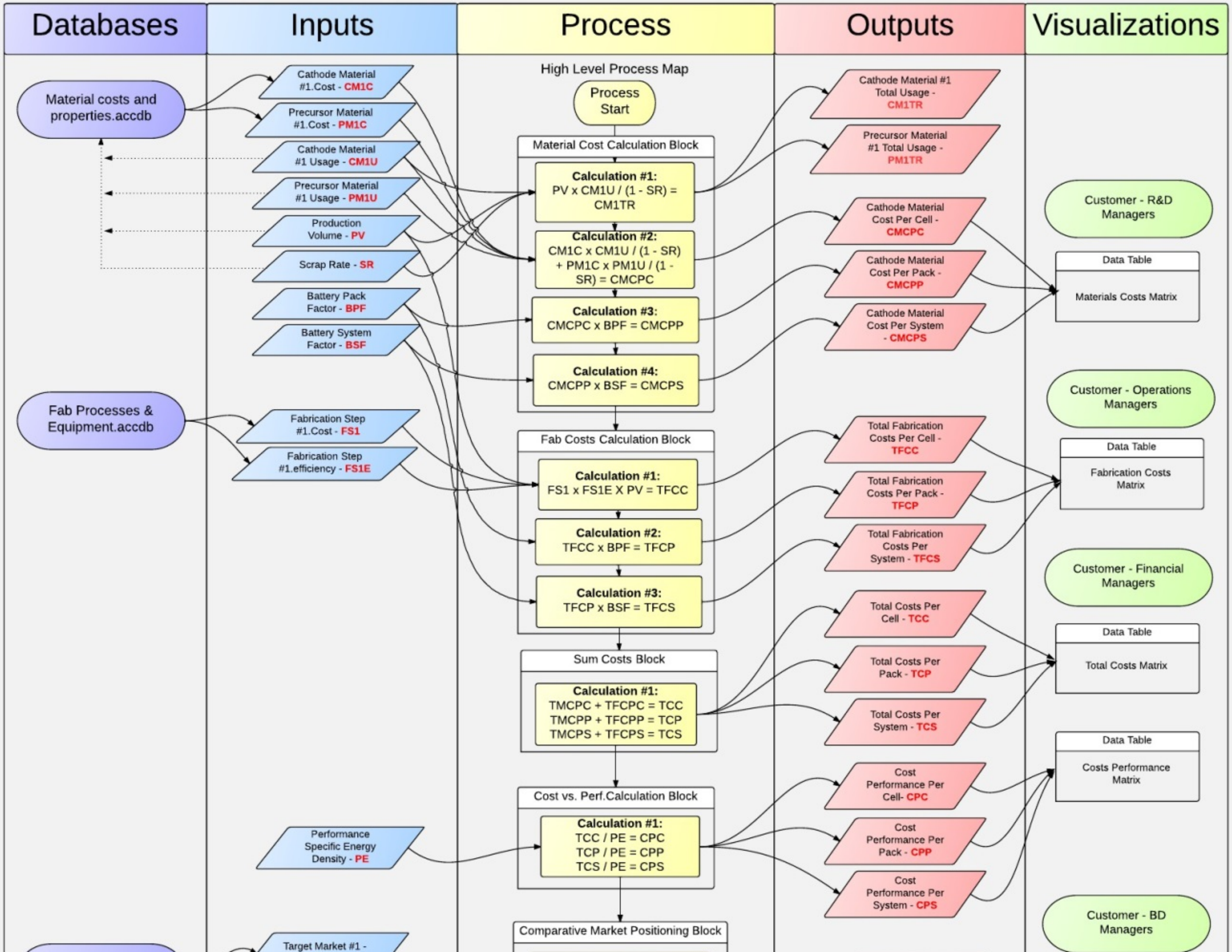


Databases
Inputs
Process
Outputs
Visualizations
Material costs and properties.accdb
Fab Processes & Equipment.accdb
Cathode Material #1.Cost - CM1C
Precursor Material #1.Cost - PM1C
Cathode Material #1 Usage - CM1U
Precursor Material #1 Usage - PM1U
Production Volume - PV
Scrap Rate - SR
Battery Pack Factor - BPF
Battery System Factor - BSF
Fabrication Step #1.Cost - FS1
Fabrication Step #1.efficiency - FS1E
Performance Specific Energy Density - PE
Target Market #1 -
High Level Process Map
Process Start
Material Cost Calculation Block
Calculation #1: PV x CM1U / (1 - SR) = CM1TR
Calculation #2: CM1C x CM1U / (1 - SR) + PM1C x PM1U / (1 - SR) = CMCPC
Calculation #3: CMCPC x BPF = CMCPP
Calculation #4: CMCPP x BSF = CMCPS
Fab Costs Calculation Block
Calculation #1: FS1 x FS1E X PV = TFCC
Calculation #2: TFCC x BPF = TFCP
Calculation #3: TFCP x BSF = TFCS
Sum Costs Block
Calculation #1: TMCPC + TFCPC = TCC TMCPP + TFCPP = TCP TMCPS + TFCPS = TCS
Cost vs. Perf.Calculation Block
Calculation #1: TCC / PE = CPC TCP / PE = CPP TCS / PE = CPS
Comparative Market Positioning Block
Cathode Material #1 Total Usage - CM1TR
Precursor Material #1 Total Usage - PM1TR
Cathode Material Cost Per Cell - CMCPC
Cathode Material Cost Per Pack - CMCPP
Cathode Material Cost Per System - CMCPS
Total Fabrication Costs Per Cell - TFCC
Total Fabrication Costs Per Pack - TFCP
Total Fabrication Costs Per System - TFCS
Total Costs Per Cell - TCC
Total Costs Per Pack - TCP
Total Costs Per System - TCS
Cost Performance Per Cell- CPC
Cost Performance Per Pack - CPP
Cost Performance Per System - CPS
Customer - R&D Managers
Data Table
Materials Costs Matrix
Customer - Operations Managers
Data Table
Fabrication Costs Matrix
Customer - Financial Managers
Data Table
Total Costs Matrix
Data Table
Costs Performance Matrix
Customer - BD Managers

Cost Model: Catalyst Layer Materials

- **Conventional (ionomer, carbon based)**
- 3M Nanostructure Thin Film (ionomer free, non-carbon)
- Hierarchical (uniform) Nanostructure (ionomer free, non-carbon)

Pt loading level: 0.15 (0.1+0.05) and 0.25 (0.2+0.05) mgPt/cm2

Conventional: Sputtering, role-based

- Direct application of Pt/C deposited on PEM (CCM) or GDL (GDE)
- Advantage: Easy to control, cheap
- Disadvantage: Low power density at low Pt loading
- Estimated cost at 100,000 production rate: **8.3 $/kW** (DOE)

NSTF (3M): Whisker formation + Pt deposition + role-to-role transfer

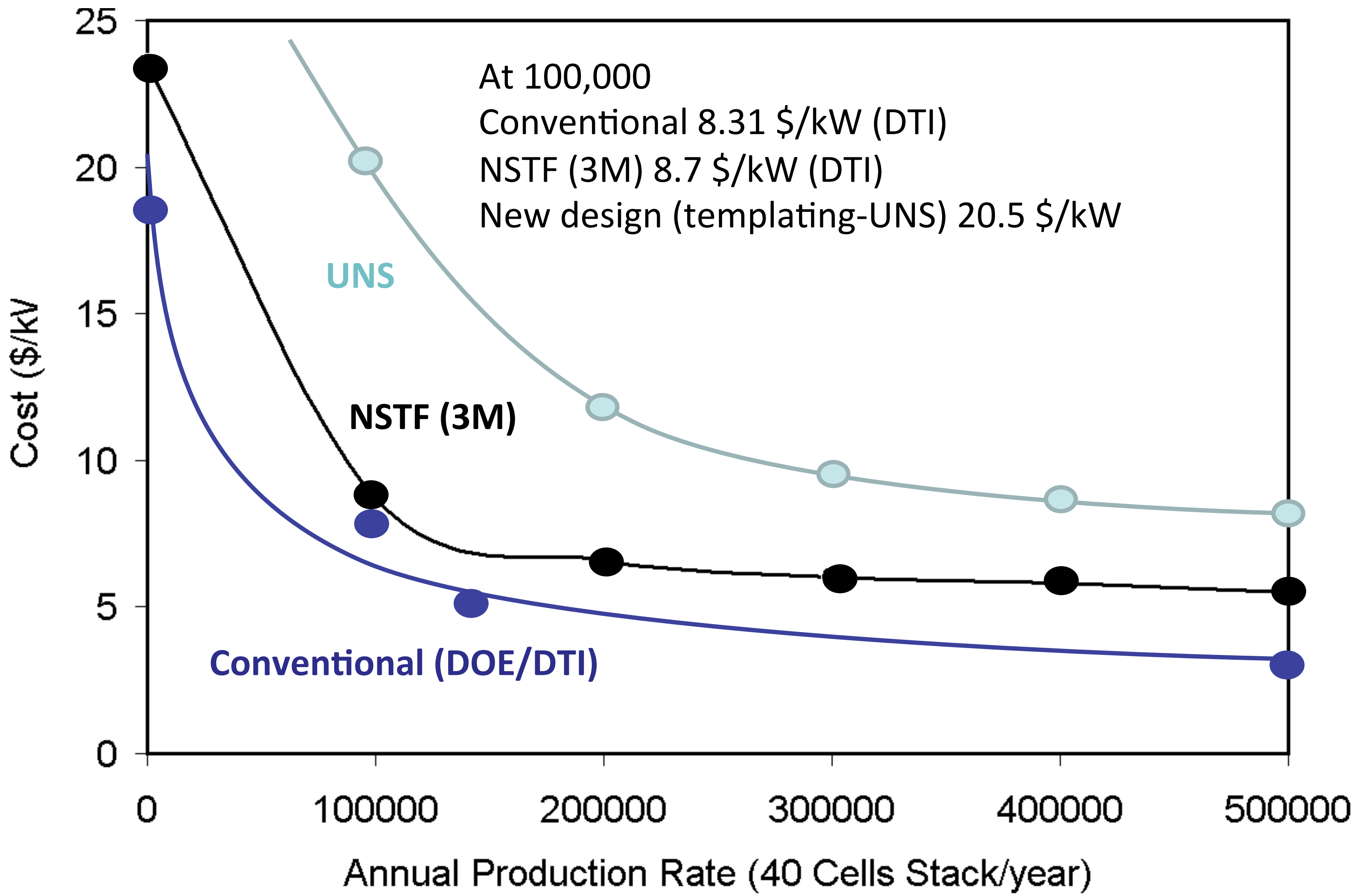
- Deposition
- Annealing
- Catalyst Sputtering
- Catalyst Transfer

Advantage: High Power at low Pt loading

Disadvantage: Need for continuous Pt phase (nonconductor support)

Estimated cost at 100,000 production rate: **8.7 $/kW** (DTI/DOE)

(Stack) Production Cost for Catalyst Layer Design



Source: Malek, Maine, Navessin, Eikerling, ESC Transaction, 2012

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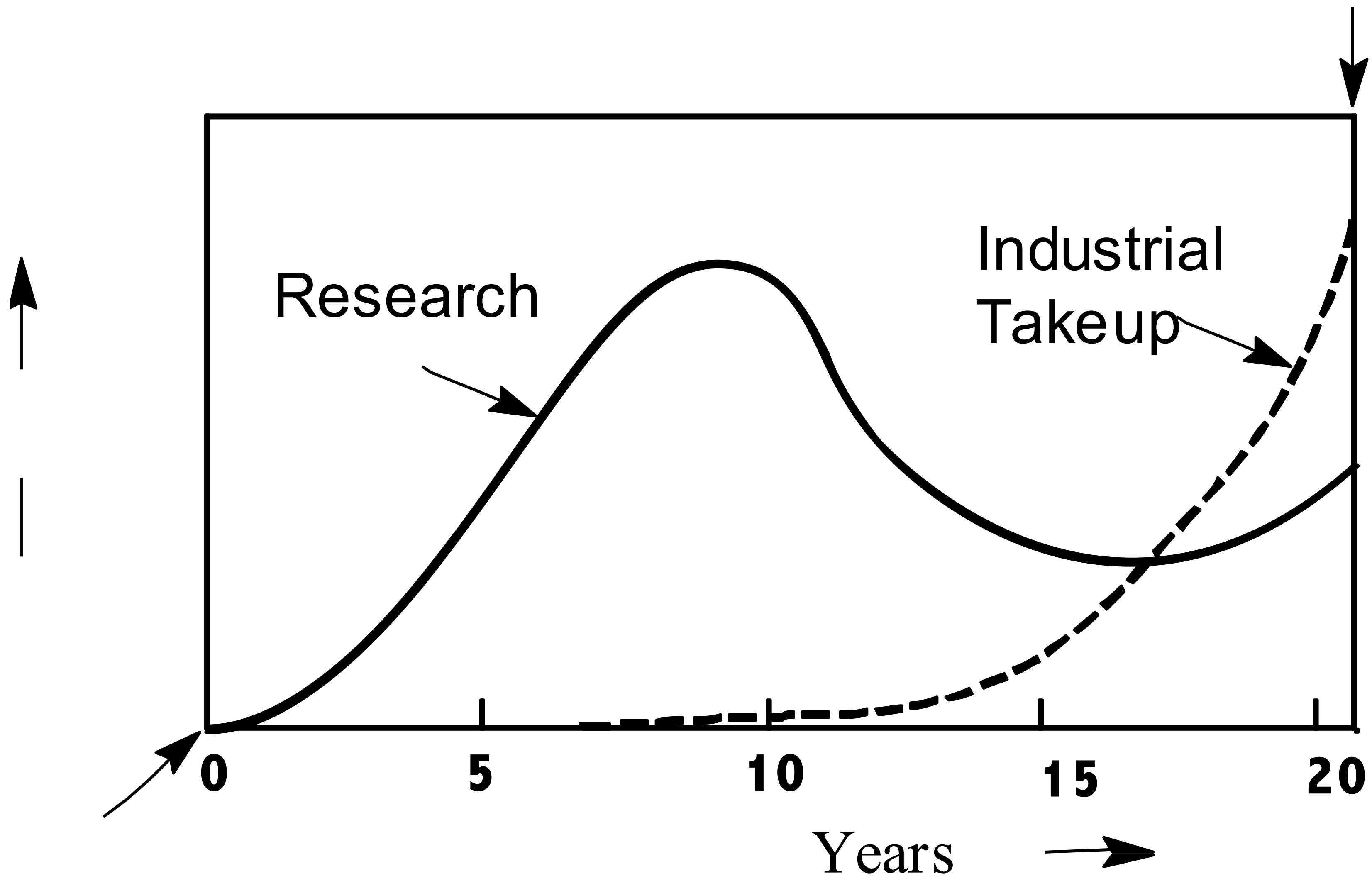
Investment & Commercialization

Adoption delays in science based innovation



Source: Maine and Ashby, 2000

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R&D Stages in New Materials Commercialization

Synthesis and Characterization

- Focus on improved functional properties
- Microstructure

Processing / Production Development

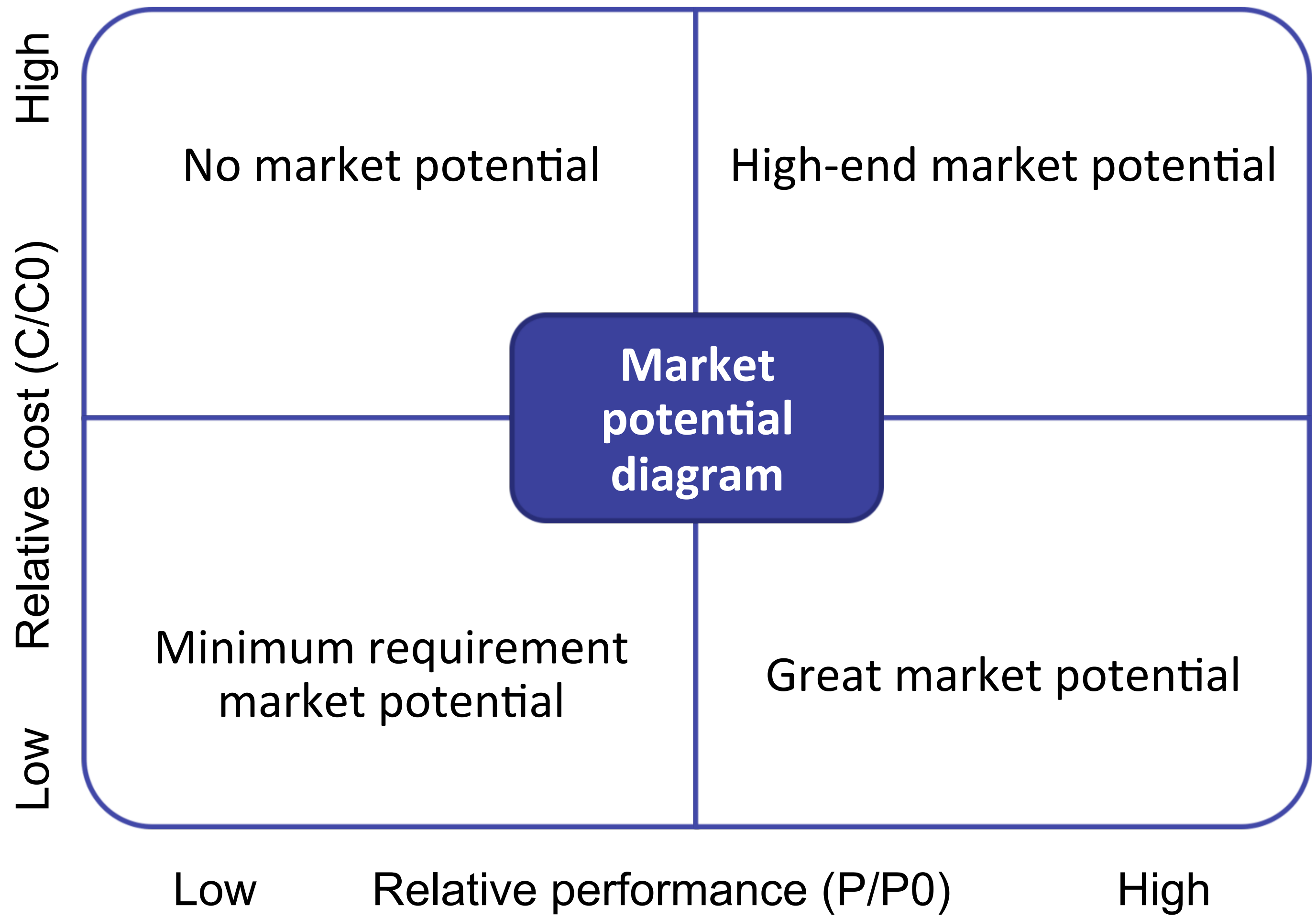
- Cost reduction
- Retain microstructure properties

Specific Development

- Regulatory approval
- Safety

Sources: Utterback, 1994, F. Maine, E. Maine

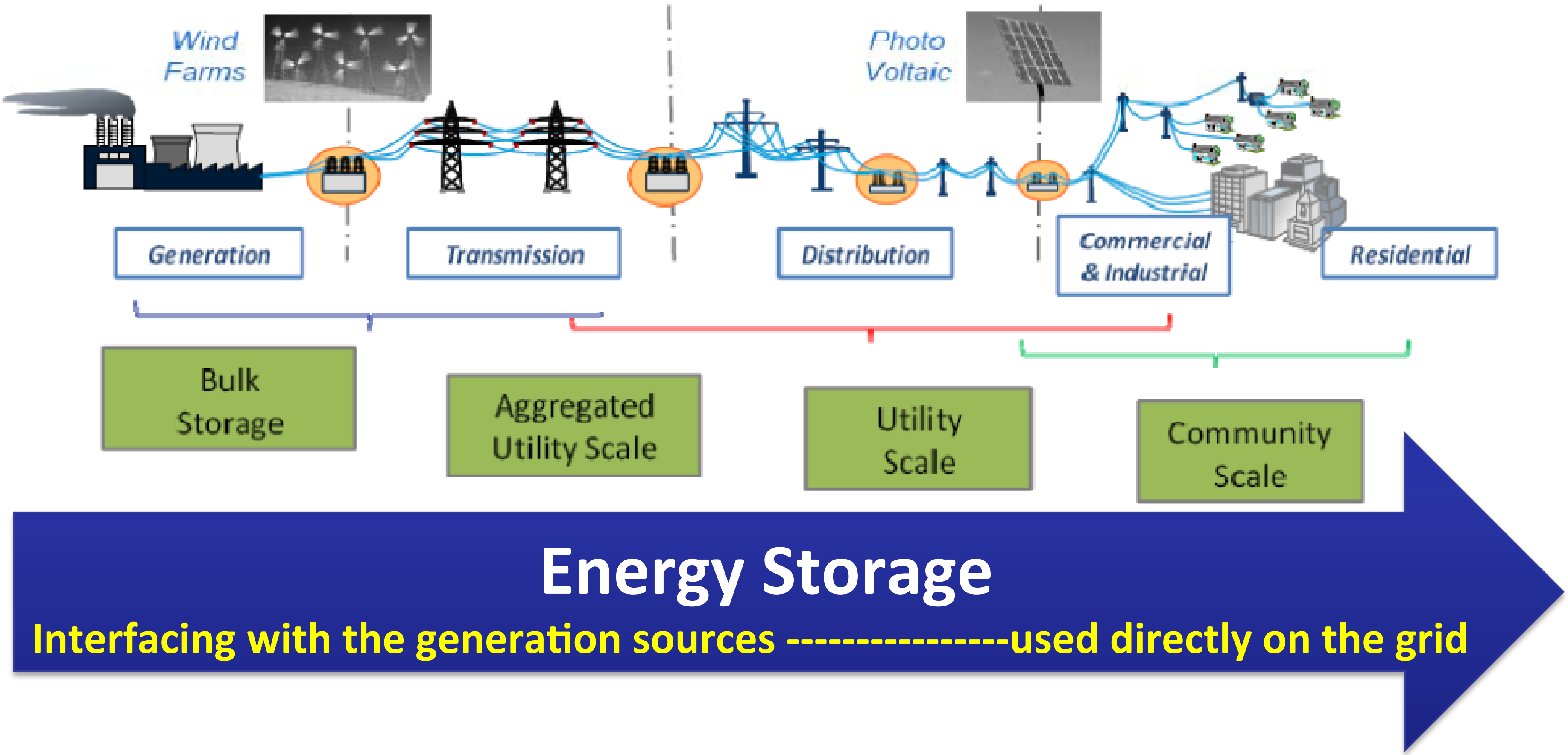
Investment Methodology for Materials (IMM)



Sources: K. Malek, E. Maine, 2012, PICMET

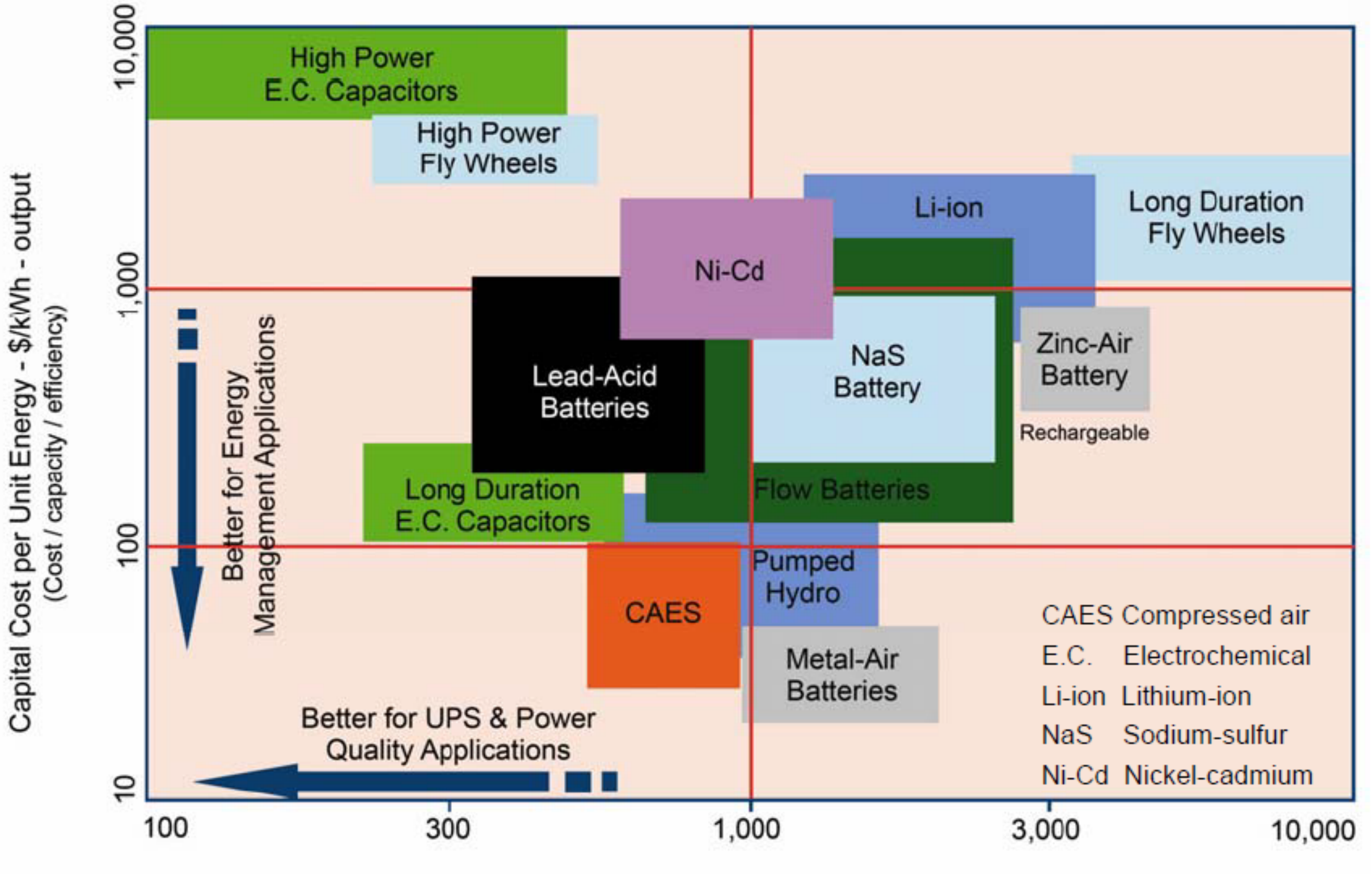
LARGE-SCALE STORAGE FOR RENEWABLE ENERGY

Grid-scale Storage Value Chain



Utility scale centralized application	Consumption Residential / commercial scale

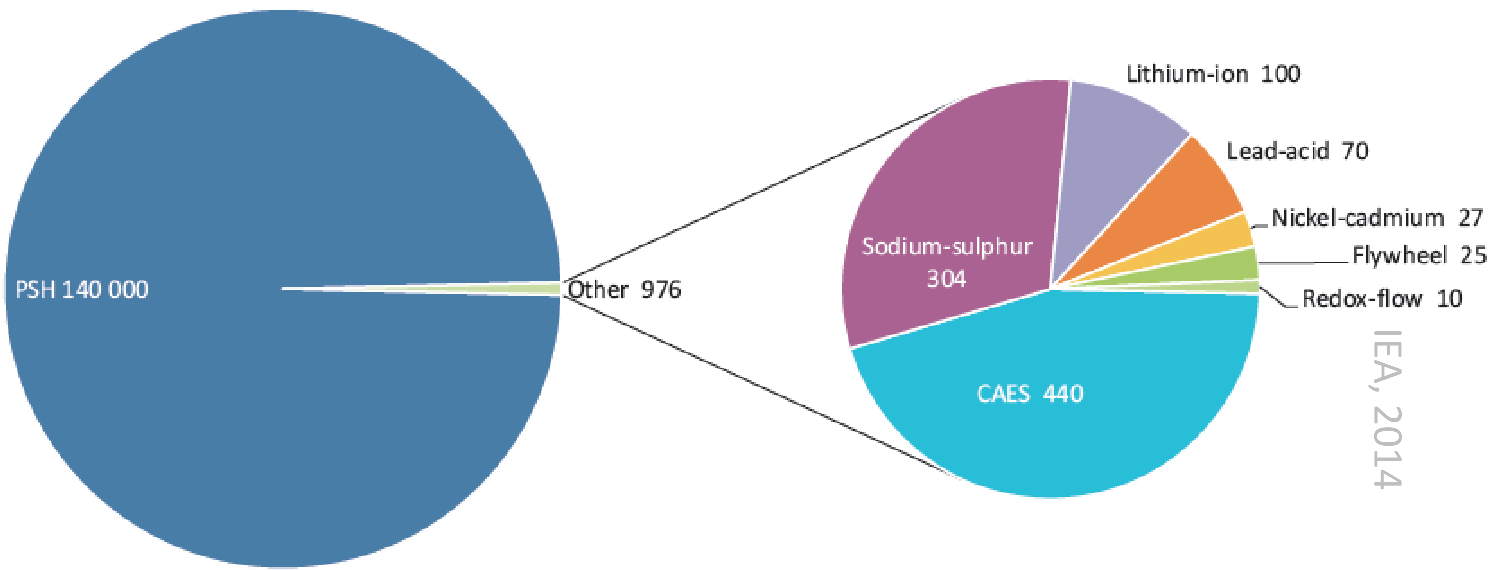
Capital cost estimation



KEMA 2011

Motivation

- Increasing role of **renewable sources** in global electricity market
- **Intermittency** of primary **renewable sources** is a limitation
- Enhancing **asset utilization rate** and **reliability** of power grids
- Energy storage as a **versatile solution**



Current grid-scale storage technologies

- NO single ES technology meets all the requirements
- Cost of storage: Lifetime and technology risks
- Life time in practical applications (not enough data yet)
- Risk of investment

Automotive: Lifetime can be increased by operating over a portion of full charge range: 1000 cycles to 80% DoD (element energy, 2012)

Not the case for ES on grid!

- Safety and standard
- 3-6 hrs of storage time is optimum for both bulk and distributed
- When energy increased the value of ES reduced, so coupled power-energy is needed at high energy applications
- Control is important: maximizes lifetime and value
- Relationships between lifetime, duty cycle, control, choice of storage technology

Materials design, component/cell performance, durability, cost

Valuing storage technologies

Generation
Power quality
Usage as energy arbitrage

→

Transmission
Investment deferral
Congestion relief
Frequency regulation

→

Distribution
Load following Power quality
Frequency regulation

→

Consumption
TOU cost reduction
Power quality

Benefit: Pricing & load data

$$\pi = Revenue - Cost$$

Cost: Technical & operational data

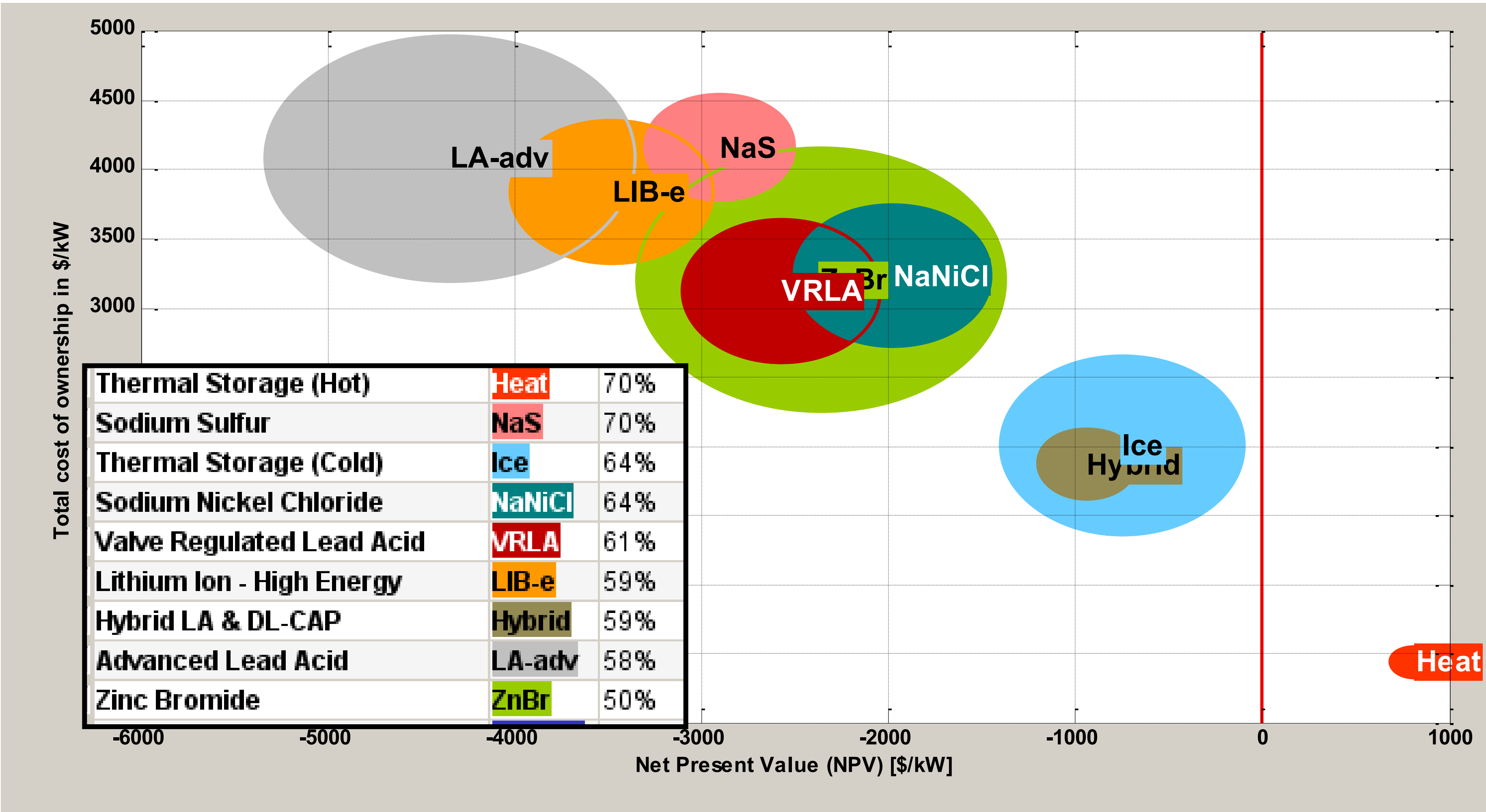
Capital cost → O&M cost → Charging cost → Taxes

Storage data-base

	Storage Technology	Abbreviations	Discharge Duration (hours) LO	Discharge Duration (hours) HI	Specific Energy (kWh/ton-metric) LO	Specific Energy (kWh/ton-metric) HI	Energy Density (kWh/m³) LO	Energy Density (kWh/m³) HI	Cycle Life at 80% DoD (1,000 cycles) LO	Cycle Life at 80% DoD (1,000 cycles) HI	Cycle Life at 10% DoD (1,000 cycles) LO	Cycle Life at 10% DoD (1,000 cycles) HI	Round Trip AC Energy Efficiency at Rated Power and 80% DoD LO	Round Trip Energy Efficier Rated Power 80% DoD HI
1	Lithium ion - High Power	LIB-p	0.2500	1	60	90	60	90	4	8	60	110	0.8400	0.9
2	Lithium Ion - High Energy	LIB-e	1	4	80	120	90	130	3.5000	7	50	100	0.8500	0.9
3	Ni batt. (NiCd, NiZn, NiMH)	Ni-batt	0.3000	3	50	90	40	210	1	3	1	3	0.7000	0.8
4	Advanced Lead Acid	LA-adv	2	5	18	30	30	70	1.2000	2.4000	20	30	0.8000	0.9
5	Valve Regulated Lead Acid	VRLA	2	4	18	25	30	60	0.6000	1	2	4	0.6800	0.7
6	Vanadium Redox Battery	VRFB	3	5	8	11	15	21	6	8	160	200	0.5800	0.6
7	Adv.Vanadium Red. Flow Batt.	A-VRFB	3	6	17	21	25	30	6	8	160	200	0.6500	0.7
8	Zinc Bromide	ZnBr	2	4	30	50	30	45	1.5000	2.5000	15	25	0.6200	0.7
9	Sodium Sulfur	NaS	6	7	80	140	100	170	5	6	40	50	0.7300	0.8
10	Sodium Nickel Chloride	NaNiCl	2	4	100	150	170	190	3	5	50	100	0.8200	0.8

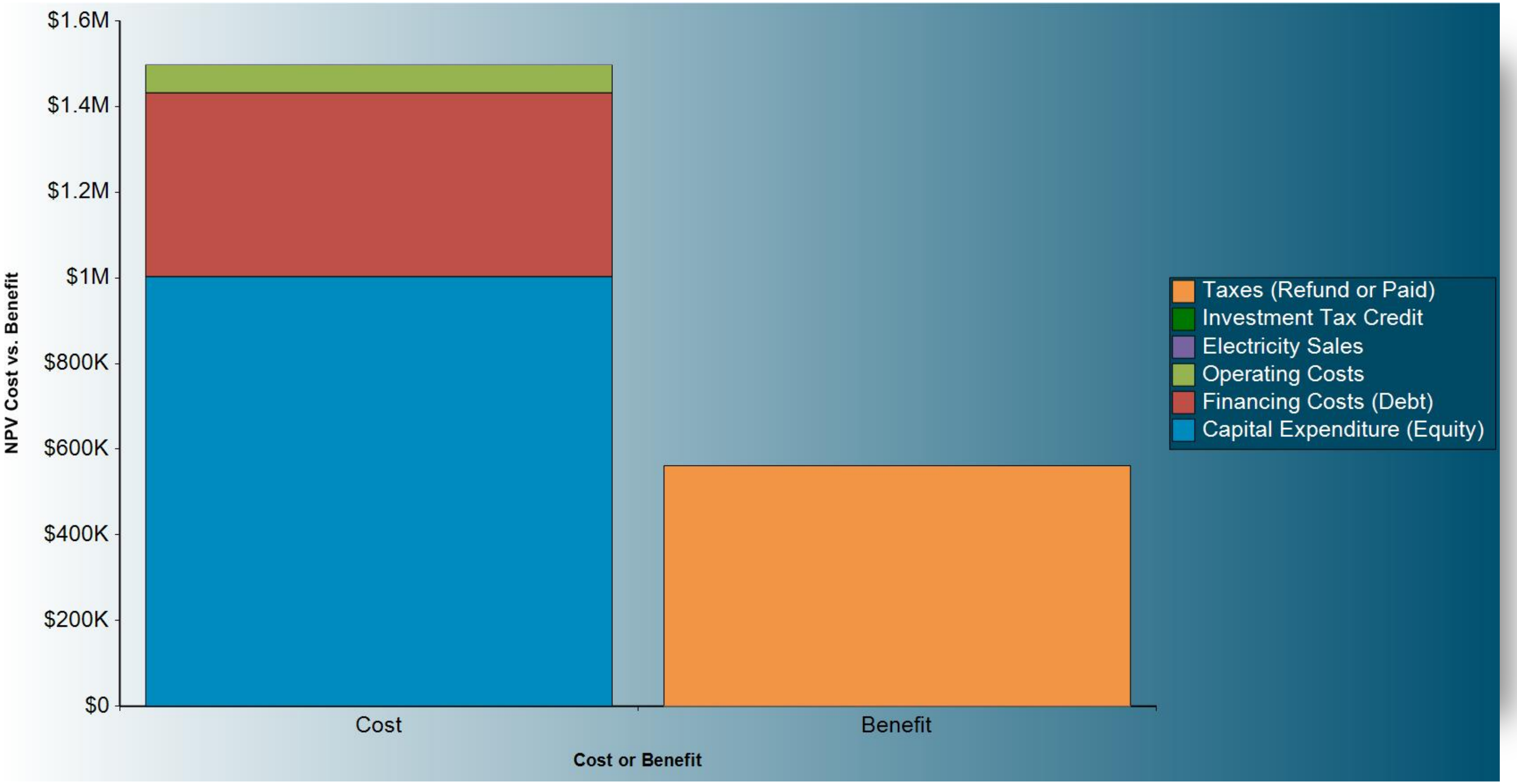
- Discharge duration (hours)
- Specific energy (kW/Ton-metric)
- Energy density (kWh/m3)
- Round-Trip AC (efficiency at 80% DoD)
- Response time to full power (s or ms)
- Footprint (m2/MWh)

NPV vs. TCO



5000
4500
4000
3500
3000
Total cost of ownership in $/kW
LA-adv
NaS
LIB-e
VRLA
NaNiCl
Ice
Heat
Thermal Storage (Hot) Heat 70%
Sodium Sulfur NaS 70%
Thermal Storage (Cold) Ice 64%
Sodium Nickel Chloride NaNiCl 64%
Valve Regulated Lead Acid VRLA 61%
Lithium Ion - High Energy LIB-e 59%
Hybrid LA & DL-CAP Hybrid 59%
Advanced Lead Acid LA-adv 58%
Zinc Bromide ZnBr 50%
-6000
-5000
-4000
-3000
-2000
-1000
0
1000
Net Present Value (NPV) [$/kW]

Case-study: Li-eB System



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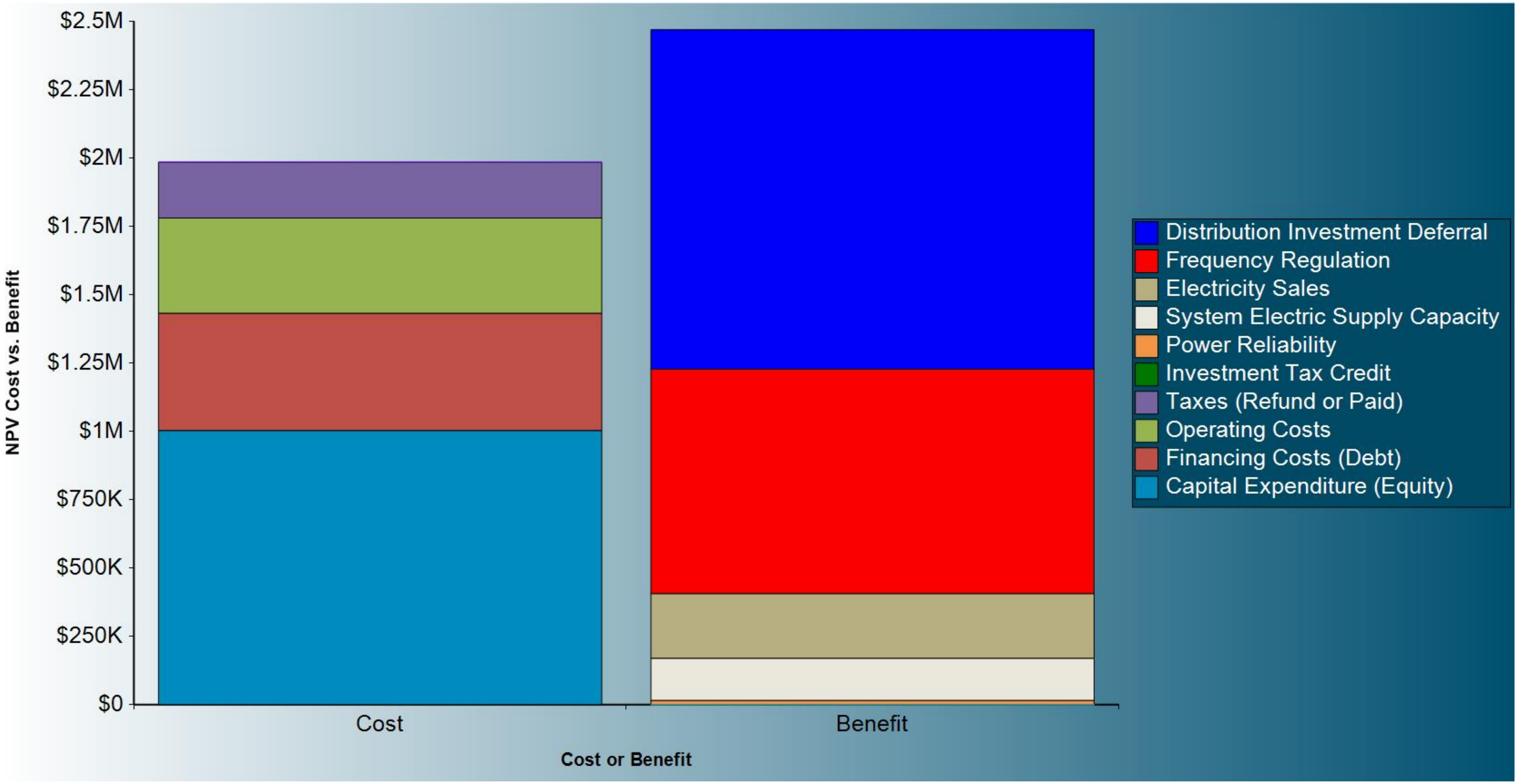


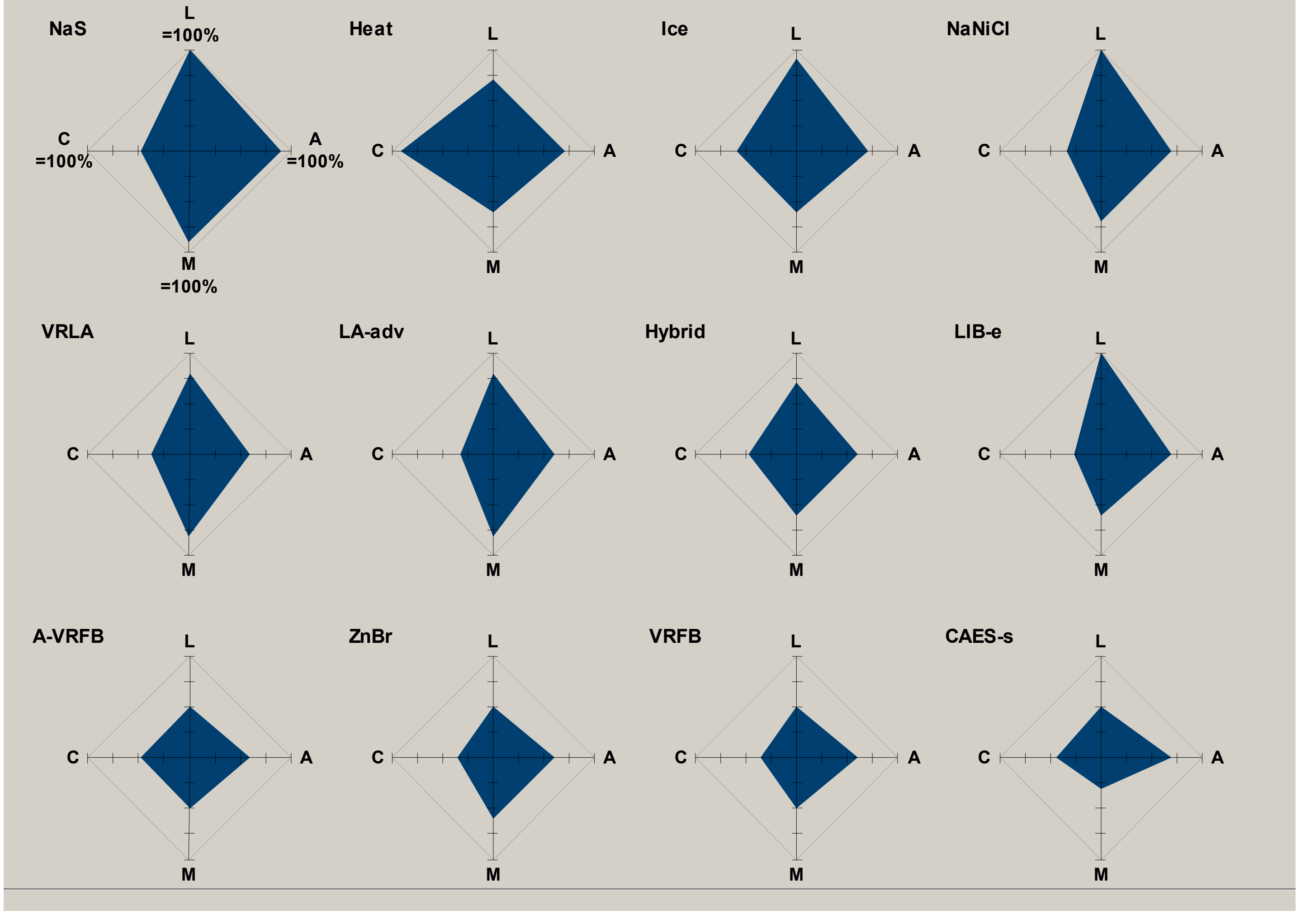
Scoring

Score for Meeting **A**pplication Requirements

Score for Meeting **L**ocation Requirements

Score for Total Installed **C**ost at Selected Location

Score for Commercial **M**aturity



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"Major regulatory hurdles must be met before storage can even be considered for use in some market……**no cohesive plan exists as to how storage technologies will be incorporated into the grid**. In addition the current system does not credit the value of storage across the entire value chain…. **The resulting challenge is the complete lack of a cost recovery system**, and with no clear path for cost reimbursement. Most utilities have open not to invest in energy storage. **It is easier for utilities to make investment in conventional approaches to addressing grid instability, such as natural gas spinning reserves, as these Investments are sure to be covered by the regulatory rate base.**"

Pike Research, 2009; Electricity Advisory Council

“Today’s consumers are expecting INNOVATION at no extra cost”

Energy Materials: Competitive advantage

A balancing act …

- Physical properties of materials
- Technical performance (components)

- Cost of production

(material, device, system)

- Market value
- Investment potential

Conclusion

- Solving the technological challenges is not enough
- Need to reduce and manage uncertainty through modeling and commercialization strategies
- Cost modeling helps to
  - Reduce uncertainty
  - Inform strategic R&D decisions
  - Determine application platform
  - Landscape mapping and best market opportunity
  - Prioritize R&D objectives, synthesis methodologies

Acknowledgement

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ÉGIDE

NISSAN

NOUS SOMMES PRETS

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Thank you

Kourosh Malek, PhD MBA
ES Program Technical Leader & Adjunct Professor
T: 604-221-3000 x5501
E: kourosh.malek@nrc.gc.ca; kmalek@sfu.ca
www.nrc-cnrc.gc.ca